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TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 2 "Ask CAS" for self-help around the clock
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NEWS 4 SEP 01 New pricing for the Save Answers for SciFinder Wizard within
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NEWS 7 SEP 27 SWETSCAN will no longer be available on STN
NEWS 8 OCT 28 KOREAPAT now available on STN
NEWS 9 NOV 18 Current-awareness alerts, saved answer sets, and current
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NEWS 10 NOV 30 PHAR reloaded with additional data
NEWS 11 DEC 01 LISA now available on STN

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MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS STN Operating Hours Plus Help Desk Availability
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:09:45 ON 03 DEC 2004

=> file .pub

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'MEDLINE' ENTERED AT 11:10:10 ON 03 DEC 2004

FILE 'BIOSIS' ENTERED AT 11:10:10 ON 03 DEC 2004

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=> s ekins s/au

L1 29 EKINS S/AU

=> e ekins s/au

E1	3	EKINS ROGER P/AU
E2	1	EKINS ROGER PHILIP/AU
E3	29 -->	EKINS S/AU
E4	66	EKINS SEAN/AU
E5	2	EKINS W L/AU
E6	1	EKINTUMAS D/AU
E7	1	EKIRIWANG JAMES T/AU
E8	10	EKIS G/AU
E9	2	EKIS IMANTS/AU
E10	6	EKIS M/AU
E11	1	EKIS M L/AU
E12	4	EKISA E G/AU

=> s e3-4

L2 95 ("EKINS S"/AU OR "EKINS SEAN"/AU)

=> s l2 and 3d/4d-qsar and cyp2d6

'4D-QSAR' IS NOT A VALID FIELD CODE

'4D-QSAR' IS NOT A VALID FIELD CODE

L3 0 L2 AND 3D/4D-QSAR AND CYP2D6

=> s l2 and cyp2d6

L4 15 L2 AND CYP2D6

=> s l4 and (four dimensional)

L5 2 L4 AND (FOUR DIMENSIONAL)

=> d 1-2 bib ab

L5 ANSWER 1 OF 2 MEDLINE on STN

AN 2000242567 MEDLINE

DN PubMed ID: 10780267

TI Three and **four dimensional**-quantitative structure activity relationship (3D/4D-QSAR) analyses of **CYP2D6** inhibitors.

AU **Ekins S**; Bravi G; Binkley S; Gillespie J S; Ring B J; Wikel J H; Wrighton S A

CS Department of Drug Disposition, Lilly Research Laboratories, Eli Lilly and Co., Lilly Corporate Center, Indianapolis, IN 46285, USA.

SO Pharmacogenetics, (1999 Aug) 9 (4) 477-89.
Journal code: 9211735. ISSN: 0960-314X.

CY ENGLAND: United Kingdom

DT Journal; Article; (JOURNAL ARTICLE)

LA English

FS Priority Journals

EM 200005

ED Entered STN: 20000525

Last Updated on STN: 20000525

Entered Medline: 20000512

AB Three- and **four-dimensional** quantitative structure activity relationship (3D/4D-QSAR) pharmacophore models of competitive inhibitors of **CYP2D6** were constructed using data from our laboratory or the literature. The 3D-QSAR pharmacophore models of the common structural features of **CYP2D6** inhibitors were built using the program Catalyst (Molecular Simulations, San Diego, CA, USA). These 3D-QSAR models were compared with 3D and 4D-QSAR partial least squares (PLS) models which were constructed using molecular surface-weighted holistic invariant molecular (MS-WHIM) descriptors of size and shape of inhibitors. The first Catalyst model was generated from multiple conformers of competitive inhibitors (n = 20) of **CYP2D6** mediated bufurololol 1'-hydroxylation. This model demonstrated a correlation of observed and predicted Ki (apparent) values of r = 0.75. A second Catalyst model was constructed from literature derived Ki (apparent)

values (n = 31) for the inhibition of **CYP2D6**. This model provided a correlation of observed and predicted inhibition for **CYP2D6** of $r = 0.91$. Both Catalyst Ki pharmacophores were then validated by predicting the Ki (apparent) of a test set of known **CYP2D6** inhibitors (n = 15). Ten out of 15 of these Ki (apparent) values were predicted to be within one log residual of the observed value using our **CYP2D6** inhibitor model, while the literature model predicted nine out of 15 values. Similarly, 3D- and 4D-QSARs derived from PLS MS-WHIM for our dataset yielded predictable models as assessed using cross-validation. The corresponding cross-validated PLS MS-WHIM model for the literature dataset yielded a comparable 3D-QSAR and improved 4D-QSAR value. Such computational models will aid in future prediction of drug-drug interactions.

L5 ANSWER 2 OF 2 BIOSIS COPYRIGHT (c) 2004 The Thomson Corporation. on STN
AN 1999:443060 BIOSIS
DN PREV199900443060
TI Three and **four dimensional**-quantitative structure
activity relationship (3D/4D-QSAR) analyses of **CYP2D6**
inhibitors.
AU **Ekins, Sean**; Bravi, Gianpaolo; Binkley, Shelly; Gillespie,
Jennifer S.; Ring, Barbara J.; Wikel, James H.; Wrighton, Steven A.
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CS Department of Drug Disposition, Lilly Research Laboratories, Lilly
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SO Pharmacogenetics, (Aug., 1999) Vol. 9, No. 4, pp. 477-489. print.
ISSN: 0960-314X.
DT Article
LA English
ED Entered STN: 26 Oct 1999
Last Updated on STN: 26 Oct 1999
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inhibitors of **CYP2D6** were constructed using data from our
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These 3D-QSAR models were compared with 3D and 4D-QSAR partial least
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the literature dataset yielded a comparable 3D-QSAR and improved 4D-QSAR
value. Such computational models will aid in future prediction of
drug-drug interactions.

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	6.01	6.22

STN INTERNATIONAL LOGOFF AT 11:13:24 ON 03 DEC 2004